Mott-Insulator to Liquid Transition and Population Trapping in Ultracold Fermi Gases by Non-Equilibrium Modulation of the Optical Lattice

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(Dated: September 20, 2011)

An ultracold gas of interacting fermionic atoms in a three dimensional optical lattice is considered, where the lattice potential strength is periodically modulated. This non-equilibrium system is non-perturbatively described by means of a Keldysh-Floquet-Green's function approach employing a generalized dynamical mean field theory (DMFT). Strong repulsive interactions between different atoms lead to a Mott-Insulator state for the equilibrium system, but the additional external driving yields a non-equilibrium density of Floquet-states and a transition to a liquid or conducting state.

PACS numbers:

In condensed matter physics quantum dynamics can only be analyzed with the premise of severe influences due to strong coupling to the environment in the experimental situation. This aspect makes it challenging to prepare bare quantum states far-from-equilibrium in a controlled way. Thus ultracold gases are wonderful systems to study the pure influences of quantum non-equilibrium effects in first instance, since the properties of such systems can be tuned almost without restrictions. At this point the reader might ask the question "Why *non*-equilibrium ?". Whereas calculations in thermodynamically equilibrated systems are well established in theory and rather complicated structures requiring high-end numerics can be solved, it is still a challenge to determine results for driven systems [1]. Nevertheless those systems are experimentally and technologically interesting [2, 3]. Even if a system is in the steady-state regime, it still not resides in thermodynamical equilibrium if it is driven *e.g.* by a nonzero current or a difference in the potential [4], and the reflection of that fact in theory is highly desirable. Besides that aspect it is a prestigious and intriguing aim to investigate fascinating quantum properties such as quantum entanglement and the onset of decoherence and dephasing [5–12] which have been measured experimentally with spectacular results.

Recently, intriguing experiments on non-equilibrium dynamics of ultracold gases, both fermionic as well as bosonic, [13–18] have become possible. Among many aspects, also the long time limit of such non-equilibrium systems has been studied [19–21], and applications using the non-equilibrium processes as a tool for transport in so called quantum ratchets have been investigated [22].

The Hubbard Hamiltonian is one of the most relevant models for investigating strongly correlated systems in condensed matter theory, of both, bosonic as well as fermionic nature [23–25]. In this Letter we study the characteristics of an interacting ultracold Fermi gas exposed to a periodic potential modulation of the optical lattice with a constant amplitude. This configuration corresponds to a stationary non-equilibrium state, which requires suitable techniques such as the Keldysh formalism. The periodic modulation leads to a 'dressing' of atoms well known from the application of light fields in quantum optics. We discuss a dynamical mean field theory (DMFT) solution for the Floquet-Keldysh [26] approach. The non-equilibrium caused dressed states arise as Floquet side-bands. In the Mott-Hubbard-gap we derive a complicated modulation induced structure of many particle states, and therefore a transition from the Mott insulting regime to a liquid phase which leads to a finite conductivity. The occupation number for these gap states is investigated and we find a trapping of population which results in an 'inversion' for increasing modulation frequencies.

The Fermi gas in the modulated optical potential is schematically shown in Fig. 1. The Mott-insulator state in equilibrium is characterized by a tight binding model

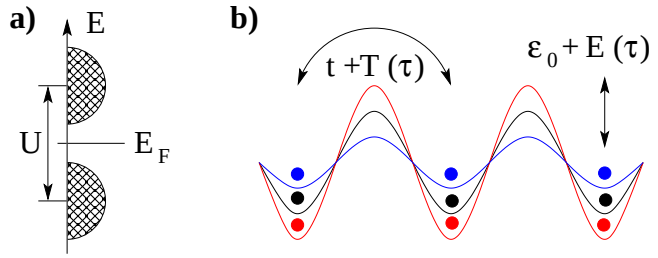

FIG. 1: (Color online) (a) The strong local interaction U between atoms in the equilibrium system, causes the single energy band to split into the lower and the upper Hubbard band, separated by an excitation gap. (b) Ultracold fermionic atoms in a 3 dimensional optical lattice (black). The optical lattice is periodically modulated with the frequency Ω_L, yielding a minimum (red) and a maximum (blue) potential modulation. The periodic modulation introduces an additional, time dependent contribution to the local atom energy $E(\tau)$ and the atomic tunneling amplitude $T(\tau)$, see text. The sketched potentials of this non-equilibrium system, therefore represent three different snapshots in time of the external periodic modulation.

with strong repulsive onsite interactions U which result in a band splitting and the establishment of the characteristic Mott-Hubbard-gap. The periodic modulation of the optical lattice potential influences the behavior of tunneling t from lattice site to the nearest neighbor as well as the onsite energies ϵ_0 at each lattice site, because these quantities depend on the lattice potential $V(\tau)$. The equilibrium tunneling amplitude t must be replaced by $t + T(\tau)$, as well as the equilibrium onsite energy has to be replaced by $\epsilon_0 + E(\tau)$. These time τ dependent terms are periodic themselves. Therefore, we consider the following Fermi-Hubbard-Hamiltonian

$$\begin{aligned} H(\tau) &= \sum_{i,\sigma} \left[\epsilon_0 + E(\tau)\right] c^\dagger_{i,\sigma} c_{i,\sigma} \qquad (1) \\ &- \sum_{\langle ij\rangle,\sigma} \left[t + T(\tau)\right] c^\dagger_{i,\sigma} c_{j,\sigma} + \frac{U}{2} \sum_{i,\sigma} c^\dagger_{i,\sigma} c_{i,\sigma} c^\dagger_{i,-\sigma} c_{i,-\sigma} \end{aligned}$$

The Index i labels the lattice site and σ the spin, $\langle ij\rangle$ implies summation over nearest neighbores, $c^\dagger_{i,\sigma}$ and $c_{i,\sigma}$ create (annihilate) a fermionic atom with spin σ at lattice site i. The time dependent contributions due to the periodic modulation of the potential are given by

$$E(\tau) = E\cos(\Omega_L \tau) \qquad T(\tau) = T\cos(\Omega_L \tau) \qquad (2)$$

where Ω_L is the frequency of the lattice modulation, τ is the system time and E and T are the respective amplitudes of energy and hopping or tunneling contribution.

The appropriate technique to describe this periodically driven system far off thermodynamical equilibrium, combines both the Keldysh [27] and the Floquet [26] Green's function approach. Due to the non-equilibrium character the Green's function truly depends on two time arguments, and the following two-time Fourier transform is employed

$$\begin{aligned} G^{\alpha\beta}_{m\,n}(\mathbf{k},\omega) &= \int_{-\infty}^{+\infty} \mathrm{d}\tau_{rel} \frac{1}{\mathcal{T}} \int_{-\mathcal{T}/2}^{+\mathcal{T}/2} \mathrm{d}\tau_{cm} e^{i(\omega - \frac{m+n}{2}\Omega_L)\tau_{rel}} \\ &\times e^{i(m-n)\Omega_L \tau_{cm}} G^{\alpha\beta}_{\sigma}(\mathbf{k}, \tau_{rel}, \tau_{cm}), \qquad (3) \end{aligned}$$

where m, n are the Floquet-indices labeling the Floquet-modes of the system, which are interpreted as quantized lattice oscillations, the phonons. Therefore the system is constrained to absorb and emit energy only in multiples of energy quanta $\hbar\Omega_L$. The Keldysh indices are $\alpha, \beta = \pm$ indicating the branch of the Keldysh contour and $\mathcal{T} = \frac{2\pi}{\Omega_L}$ is the time period. The system time is shifted to a center of motion time $\tau_{cm} + \frac{\tau_1 + \tau_2}{2}$ and a relative time coordinate $\tau_{rel} = \tau_1 - \tau_2$. For completeness and later comparison, we note that for the non-interacting case, *i.e.* $U = 0$ the Hamiltonian Eq. (1) can be solved analytically, yielding

$$G^R_{mn}(\mathbf{k},\omega) = \sum_{\rho=-\infty}^{\infty} \frac{J_{\rho-m}\left(\frac{E}{\Omega_L} + T\frac{\tilde{\epsilon}_\mathbf{k}}{\Omega_L}\right) J_{\rho-n}\left(\frac{E}{\Omega_L} + T\frac{\tilde{\epsilon}_\mathbf{k}}{\Omega_L}\right)}{\omega - \rho\Omega_L - \epsilon_\mathbf{k} + i\mathcal{O}}. \qquad (4)$$

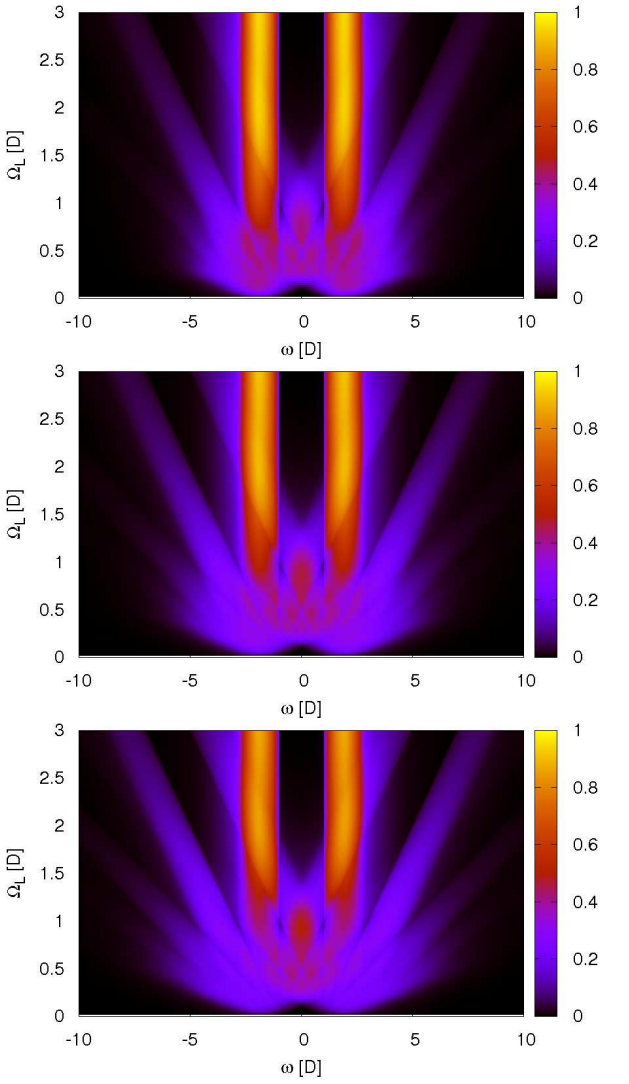

FIG. 2: (Color online) The local density of states (LDOS) given by $\sum_n \mathrm{Im}\, G^R_{0\,n}(\omega)$ for the non-equilibrium systems characterized by $T = 2.0, 3.0, 4.0$ (from top to bottom), for $U = 4.0$ and $E = 1.0$. The LDOS is displayed as a function of atomic energies ω and lattice modulation frequencies Ω_L, D is the half bandwidth.

We note that $\epsilon_\mathbf{k}$ is the dispersion induced by the standard hopping t, and $\tilde{\epsilon}_\mathbf{k}$ originates from the modulation induced hopping contribution $T(\tau)$, ρ is the integer summation index. To solve the full, *i.e.* driven and interacting system ($U \neq 0$) at zero temperature and half filling, we generalize a non-equilibrium dynamical mean field theory (DMFT) [28]. The DMFT maps the interacting system onto a local impurity model [29, 30], which is solved here by iterated perturbation theory (IPT) technique [31], which is a diagrammatic method and has also been generalized for non-equilibrium systems. This substantial numerical effort results in the full knowledge of the non-equilibrium Floquet-Keldysh-Green's function, revealing *e.g.* the local density of states

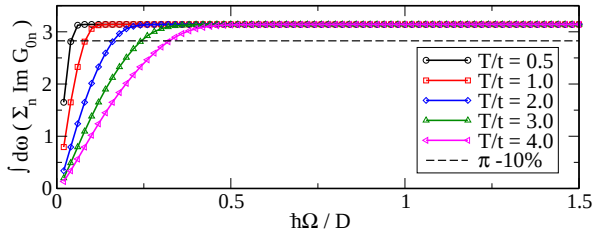

FIG. 3: (Color online) Shown is the ω and $\mathbf{k}$ integrated imaginary part of retarded component of the calculated Floquet-Keldysh Green's function, *i.e.* $\int \mathrm{d}\omega \int \mathrm{d}^3k \sum_n \mathrm{Im}\, G_{0,n}(\omega, \mathbf{k})$ as a function of Ω_L for different strengths of the induced hopping T as shown, for energy $E = 1$. The onsite repulsion strength is $U = 4.0$, cf. Fig. 2. Due to numerical restrictions, the number of Floquet modes included in the actual calculations is limited. Throughout this letter we use $n = -10 \ldots + 10$, *i.e.* we include the lowest 21 Floquet modes in our calculations. This finite number introduces an error to the numerical results as $\Omega_L \to 0$. $\int \mathrm{d}\omega \mathrm{Im} G_{0,n}$ must be equal π if the solution is valid. The deviations show the range of validity. For small lattice modulation frequencies Ω_L, the numerical quality depends on the strength of the induced hopping T for a given E. For strong correlations of about $U = 4.0$, *i.e.* the corresponding equilibrium system is in the insulating regime, the deviation is less then 10% for frequencies $\Omega_L > 0.25$ which marks the prospected range of validity for the parameters used in this Letter.

(LDOS), the non-equilibrium distribution function, and the relaxation times by means of the self-energy. A solution for the LDOS is shown in Fig. 2, where we display $\mathrm{Im}\, G^R(\omega) = \int \mathrm{d}^3\mathbf{k} \sum_{m\,n} \mathrm{Im}\, G^R_{m\,n}(\omega, \mathbf{k})$. We need to account for all the emission and absorption events of externally induced energy quanta $\hbar\Omega_L$, and therefore we have to sum over all indices m, n. We set $\hbar = 1$. Furthermore all energies U, E, ϵ_0, T, t, ω and Ω_L are given in units of of half bandwidth D.

In Fig. 2 we discuss the development of pronounced

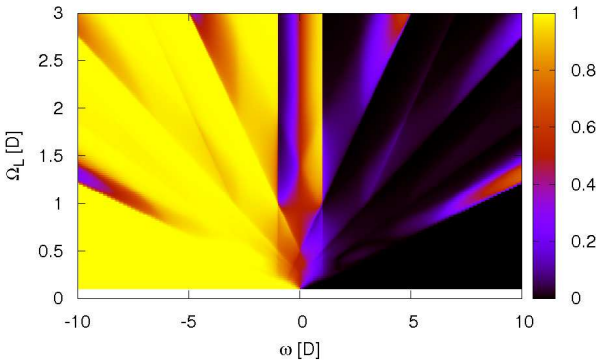

FIG. 4: (Color online) Displayed is the non-equilibrium distribution function of the fermionic ultracold gas as a function of atomic energy ω and external modulation frequency Ω_L. The parameters for this original insulating state are $U = 4.0$, $T = 2.0$ $E = 1.0$. Please note the behavior around external modulation frequencies of $\Omega_L \simeq 1$, also see text.

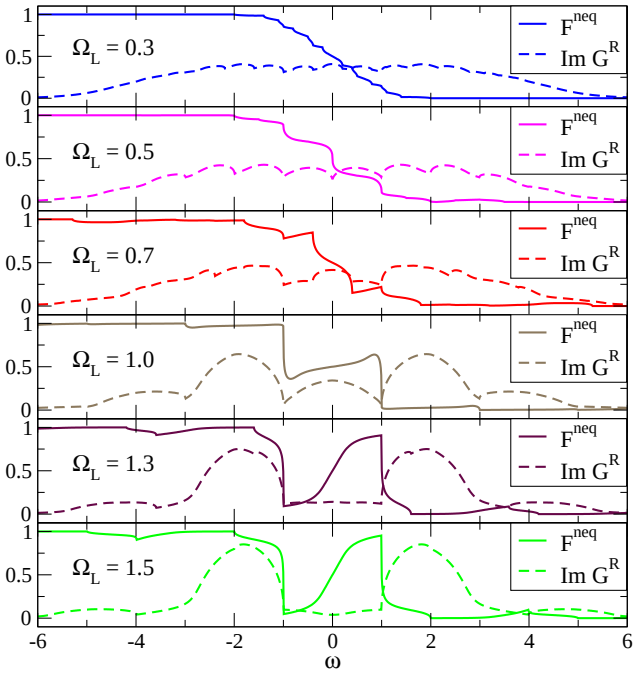

FIG. 5: (Color online) Displayed is the non-equilibrium distribution function of the fermionic gas together with the corresponding imaginary part of the retarded component of the local Green's function (DOS) for parameters $U = 4.0$, $T = 2.0$ $E = 1.0$ at a series of different external modulation frequencies , $\Omega_L \in \{0.3, 0.5, 0.7, 1.0, 1.3, 1.5\}$, from top to bottom. The band gap in equilibrium has the width $2D$. For a detailed discussion see text.

Floquet side-bands in the LDOS structure with respect to an enhancement of the hopping amplitude T. Distinct gap-states evolve which induce a transition from the Mott-insulator state to the liquid phase. Both features result in severe changes of the fermionic band structure and therefore cause significant changes of *e.g.* optical and conduction properties.

The behavior of the density of states as function of the external modulation frequency Ω_L exhibits two limiting cases with a cross-over regime between them. For the limit of small modulation frequencies $\Omega_L \to 0$ it is interesting to note that all Floquet-modes gain more and more spectral weight. This signals the onset of an orthogonality catastrophe, as predicted by P. W. Anderson (AOC) [32]. The system undergoes a transition to a new ground state which is orthogonal to the original equilibrium state, caused by the change in the potential of the system Fig. 2. Technically this is seen as drastic enhancement of the arguments of the Bessel functions, *e.g.* for the non-interacting expression in Eq. (4). Considering the behavior of the Bessel functions, we note that with decreasing modulation frequency the number of Floquet modes, which contribute, increases. Numerical calculations however are always limited to treatments regarding a finite number of Floquet modes. Therefore our numer-

ics is optimized towards the limit of maximum validity for an affordable amount of computational effort. A detailed analysis can be found in Fig. 3 and caption.

In Fig. 5 we discuss the behavior of the LDOS and the occupation number for increasing external modulation frequency Ω_L. For frequencies $\Omega_L < 1$ the behavior of the ultracold Fermi gas changes from Mott-insulating to liquid or conducting. Pronounced Floquet-side bands [26] are developed and intersect in between the Hubbard-bands. The Mott-gap almost disappears and a liquid or conducting regime is established, where the liquid density of states can be continuously driven by the external modulation. Regarding the occupation number of the gap states we find a step-like behavior for long wavelength modulations which can be interpreted as the absorption or emission of energy quanta (phonons). In the non-equilibrium fermionic distribution function we derive that for long wavelength modulations the majority of fermions resides in states below the Fermi edge ($\omega = 0$).

The two limiting regimes of small and large lattice modulations are separated by a cross-over at $\Omega_L \simeq 1$ (see Fig. 2). At the crossing, the modulation induced Floquet-side bands are forced to intersect in the gap and acquire a maximum of spectral weight (see Fig. 4) in this area. Moreover the occupancy from the states right above the lower Hubbard-band is shifted towards states right below the upper Hubbard-band and additionally the entire gap is almost equally occupied. We further remark that the excitation behavior to reach the upper Hubbard-band at the crossing changes from virtual, *i.e.* successive absorption, to direct.

Right above the crossing, for external modulation frequencies $\Omega_L > 1$ we find, that the liquid behavior is dramatically reduced. In the lower panels of Fig. 5 we discuss the LDOS and the distribution function in the for external frequencies above $\Omega_L = 1$. We have to remark that above the crossing the LDOS shows a significant change in the gap. The step-like structure vanishes and the system reveals for further increasing Ω_L almost the behavior of a Mott-insulator with an unconventional occupation number in the Mott-gap associated with a weak spectral weight there. Combining both, the discussion concerning the spectral weight and the distribution number right above $\Omega_L = 1$ we find a pronounced shift of occupation which resembles a "trapping" of particles right below the upper Hubbard-band, which is an "inversion" alike situation. The Fermions can not relaxate because no unoccupied states are within reach if we assume only emission processes of an integer number of phonons. For significantly faster lattice vibrations of the confining potential the system is not able to follow the perturbations and returns to a stationary state similar to equilibrium. The trapping of the occupation is preserved.

To conclude we discussed a theory of ultracold fermionic atoms described by a Hubbard model including strong repulsive interactions. Periodic lattice potential modulations which drive this system out of thermodynamical equilibrium were considered. By investigating a Floquet-Keldysh Green's approach we find a cross-over between two limiting characteristics, the AOC for $\Omega_L \to 0$ and a quasi-equilibrium solution for $\Omega_L \to \infty$. Pronounced side-bands lead to a rather complicated density of states in the gap for $\Omega_L < 1$ which indicates a transition to the liquid or conducting regime right at the onset of the modulation. In the vicinity of the cross-over we find a maximum of spectral weight inside the original excitation gap. For external frequencies $\Omega_L > 1$ population trapping in the gap is observed. Beyond the system approaches an equilibrium-like Mott-insulator regime which indicates that the system is not able to follow very fast perturbations.

The author thanks Andreas Lubatsch, Michael Marthaler, Allard P. Mosk and Hartmut Monien for valuable discussion. Support by the Karlsruhe School of Optics and Photonics (KSOP) is acknowledged.

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